

Multi-Scale (nano-to-device), Multi-Physics Software For Design of Nanobiosystems, Phase I

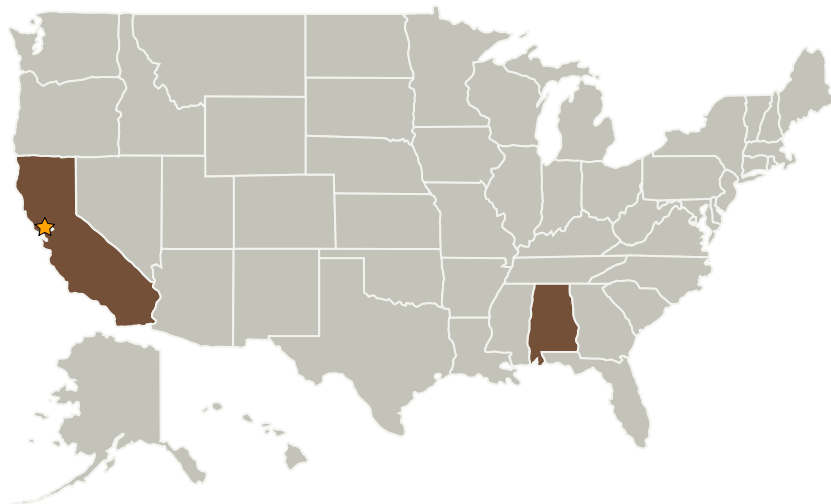
Completed Technology Project (2004 - 2004)



Project Introduction

Nanobiotechnology is a rapidly advancing frontier of science with great potential for beneficial impact on society. However, successful design of these systems is an extremely complex, laborious task with large failure rates. Current models describing the molecular behavior are too slow (nanoseconds) and expensive while device design codes lack the necessary nanophysics. Our overall objective is to develop a generalized, multiscale, multiphysics CFD (continuum)-based design software where nanoscale effects of arbitrary biosystems are accurately, efficiently and seamlessly integrated with coarse-grained models carrying molecular information. To accomplish this task we propose a three-level modeling effort. First molecular calculations (Molecular Dynamics, Monte Carlo) are undertaken to elucidate the fundamental and essential molecular behavior. Next, stochastic simulation methods (Master, Fokker-Planck, or Langevin) will be seamlessly integrated with continuum approaches are developed to describe the mesoscale, fast time scale averaged behavior of these molecules. Finally, the information from the stochastic models is coupled to the continuum CFD model. In Phase I, the feasibility of this approach will be developed and demonstrated in the context of nanopore based sequencing device. The Phase II work will focus on model generalization, validation and improved usability (speed, robustness, GUI). The research is leveraged on substantial prior effort in the area.

Primary U.S. Work Locations and Key Partners



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Organizational Responsibility

Responsible Mission Directorate:

Space Technology Mission
Directorate (STMD)

Lead Center / Facility:

Ames Research Center (ARC)

Responsible Program:

Small Business Innovation
Research/Small Business Tech
Transfer

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Organizations Performing Work	Role	Type	Location
★ Ames Research Center(ARC)	Lead Organization	NASA Center	Moffett Field, California
CFD Research Corporation	Supporting Organization	Industry	Huntsville, Alabama

Primary U.S. Work Locations

Alabama	California
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Project Management

Program Director:

Jason L Kessler

Program Manager:

Carlos Torrez

Principal Investigator:

Jerry A Jenkins

Technology Areas

Primary:

- TX09 Entry, Descent, and Landing
 - └ TX09.4 Vehicle Systems
 - └ TX09.4.5 Modeling and Simulation for EDL